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MINIMIZATION TECHNIQUES USING RATIONAL APPROXIMATIONS

By

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
MANNED SPACECRAFT CENTER
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MINIMIZATION TECHNIQUES
USING RATIONAL APPROXIMATIONS

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SUMMARY

The purpose of this paper is to present a curve fitting method using rational approximations. Curve fitting problems are frequently encountered here at the Manned Spacecraft Center. Polynomial approximations are used for a major portion of these problems because of the simplicity in applying polynomial least squares techniques directly to any set of data. Polynomial approximations are not accurate enough to be acceptable in many cases. The method developed in this paper is superior to the best least squares polynomial approximation for a large class of curves. It is well known that low order rational approximations are often as accurate as high order polynomial approximations (Ref. 1). Considerable computer time can be saved by using the low order rational approximation if a large number of points must be calculated. The rational approximation method derived herein can be applied to any set of data just as easily as least squares polynomial techniques. However, matrix inversion must be used to obtain the final result. This can, in some cases, result in undesirable round off errors which can lessen the accuracy of the method.

LIST OF SYMBOLS

$\{x_i\}$; $i = 1,N$	discrete set of values for independent real variable
$\{y_i\}$; $i = 1,N$	corresponding set of values for dependent real variable
A^T	transpose of a matrix A
A^{-1}	inverse of the matrix A
$K + 1$	number of parameters in minimization technique
$\{\alpha_i\}$; $i = 1,K$	the K parameters to be obtained for minimization

INTRODUCTION

The basic problem of curve fitting[1] is to formulate an analytical expression to replace a discrete set of data points. The analytical expression can then be used to interpolate and/or extrapolate. The need for interpolation and extrapolation occurs in numerical integration, data

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[1]The problem of curve fitting is restricted here to a discrete set of points because this is the major concern of this paper. In general the problem is extended to an infinite number of points (Ref. 2).

reduction, and engineering problems using experimental data. Examples are radiation intensity curves, the derivative of atmospheric density with altitude, and guidance control functions. Analytical expressions are preferred because computations of the analytical expression takes less time and fewer locations in memory than table look up procedures.

There are two aspects of curve fitting: (1) the smoothing of noisy data, and (2) the fitting of exact data points by an analytical expression. Only the latter aspect is discussed in this paper. If the data is exact then table look up procedures are usually more accurate near the original points.

GENERAL STATEMENT OF THE PROBLEM

A curve fitting technique can be automated in the following manner:

If (1) $\{x_i\}$ $i = 1,2,\ldots,N$ is a discrete set of independent real variables

(2) $\{y(x_i)\}$ $i = 1,2,\ldots,N$ is the corresponding set of dependent real variables.

Then choose the following:

(3) $f(x,\alpha,K) \in F$

(4) $||f(x_j,\alpha,K),\ y(x_j)||_{j=1}^{N}$

(5) $\phi\left(||f(x_j,\alpha,K),\ y(x_j)||_{j=1}^{N}\right)$

Where F is a class of functions involving $K + 1$ arbitrary parameters $(\alpha_0, \alpha_1, \ldots, \alpha_K) = \alpha$ and the functional form of f is specified.

(4) $||f,y||$ is the norm of $f(x_j, \alpha, K)$, $y(x_j)$, $j=1,\ldots,N$ which measures the accuracy of f.

(5) ϕ is an automated minimization technique which determines α such that (4) is a minimum.

Thus, if (1), (2) and K are determined, the automated technique obtains a particular α, such that for the class of functions F, $f(x,\alpha,K)$ is the most accurate function with respect to the norm chosen in (4). The choice of the norm is discussed by Rice (Ref. 3).

The major disadvantage of the automated technique is that the data points might be of such a form that, regardless of the choice of K, the best approximating function from the class F is not acceptable to the user. This usualy stems from the practical numerical problems involved in the minimization technique rather than from the theoretical basis.

LEAST SQUARES POLYNOMIAL APPROXIMATION

Least squares polynomial approximations are automated as follows:

(1) F is the class of polynomial of the form

$$f(x,\alpha,K) = \alpha_0 + \alpha_1 x + \ldots \alpha_K x^K$$

$$(2) \quad \left|\left| f(x_j,\alpha,K),\; y(x_j) \right|\right|_{j=1}^{N} = \sum_{j=1}^{N}\Big(f(x_j,\alpha,K) - y(x_j)\Big)^2$$

If K is fixed,

$$A = \{a_{ij}\} = \{x_i^{j-1}\} \qquad \begin{array}{l} i = 1,2,\ldots N \\ j = 1,2,\ldots K+1 \end{array}$$

If a minimum exists and $A^T A$ is non-singular, then there exists a unique α such that (2) is minimized. In this case α is given by

$$\alpha = (A^T A)^{-1} A^T y(x_j) .$$

RATIONAL APPROXIMATIONS

The objective of this method is to obtain a rational approximation $y(x)$ to a discrete set of data points

$$y(x) = f(x,\alpha,K) \;/\; f(x,\beta,m)$$

Milne (Ref. 1) has shown that certain classes of functions are better approximated by rational functions than by polynomials. Moreover, there are physical problems which are characterized by an underlying mathematical model which is of rational function form, (for example, the aerodynamic lift of a flat plate (Ref. 3)). However, for problems which do not have a rational function as an underlying model, the method in no way assures the best rational approximation with respect to the least squares norm.

METHOD

(1) Given a discrete set of N data points $\{y(x_i), x_i \quad i = 1,2,\ldots,N\}$ choose an integer K and apply a least squares polynomial approximation to the data such that

$$\sum_{i=1}^{N} \Big(p(x_i,\alpha,K) - y(x_i)\Big)^2$$

is a minimum.

(2) Choose two integers m , n such that $n < K$, $m + n + 2 < N$.

(3) Solve for the two polynomials $p(x, \beta,m)$, $p(x, \delta,n)$ such that

$$\sum_{i=1}^{N} \Big(p(x_i, \beta,m)\; y(x_i) + p(x_i, \delta,n) - p(x_i,\alpha,K)\Big)^2 \qquad (1)$$

is a minimum.

(4) The approximation for $y(x)$ is given by

$$y(x) \;=\; \Big(p(x,\alpha,K) - p(x, \delta,n)\Big) \,/\, p(x, \beta,m) \qquad (2)$$

The minimization of (3) can be obtained very simply as follows:

Let $A = \{a_{ij}\}$ such that

$$a_{ij} = x_i^{j-1}\, y(x_i) \qquad \begin{array}{l} j = 1,2,\ldots,m+1 \\ i = 1,2,\ldots,N \end{array}$$

$$a_{ij} = x_i^{j-(m+2)} \qquad \begin{array}{l} j = m+2,\ldots,m+n+2 \\ i = 1,2,\ldots,N \end{array}$$

If A^TA is nonsingular then the solution is unique and is given by

$$\begin{Bmatrix} \beta_0 \\ \beta_1 \\ . \\ . \\ . \\ \beta_m \\ \delta_0 \\ \delta_1 \\ . \\ . \\ . \\ \delta_n \end{Bmatrix} = (A^TA)^{-1} A^T \begin{Bmatrix} p(x_1,\alpha,K) \\ p(x_2,\alpha,K) \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ . \\ p(x_N,\alpha,K) \end{Bmatrix}$$

Theorem: If there exists a rational function such that

$$y(x_i) = p(x_i,r,K) \,/\, p(x_i,\varepsilon,m) \qquad (3)$$

$$i = 1,2,\ldots,N$$

then the preceding method is exact (to within round off error), provided $m = K - 1$

Proof:

If $p(x,\alpha,K)$ is the least squares polynomial approximation to x_i, $y(x_i)$ then consider δ_i such that

$$\frac{r_i}{\delta_i - \alpha_i} = \frac{r_K}{\alpha_K} \qquad i = 1,2,\ldots,K - 1$$

Then

$$\frac{p(x,r,K)}{p(x, \delta, K - 1) - p(x,\alpha,K)} = \frac{r_K}{\alpha_K}$$

thus, there exists $p(x, \delta, K - 1)$ such that

$$p(x, \delta, K - 1) - p(x,\alpha,K) = \frac{\alpha_K}{r_K} p(x,r,K)$$

Also consider $\beta_i \quad i = 1,2,\ldots,m$

such that

$$\beta_i = - \frac{\alpha_K}{r_K} \varepsilon_i$$

Thus, there exists $p(x,\beta,m)$ such that

$$p(x,\beta,m) = - \frac{\alpha_K}{r_K} p(x,\varepsilon,m)$$

But this implies that, by (1)

$$p(x,\beta,m)\ y(x) + p(x,\ \delta,\ K-1) - p(x,\alpha,K) =$$

$$-\frac{\alpha_K}{r_K}\ p(x,\varepsilon,m)\ \frac{p(x,r,K)}{p(x,\varepsilon,m)} + \frac{\alpha_K}{r_K}\ p(x,r,K) =$$

$$-\frac{\alpha_K}{r_K}\ p(x,r,K) + \frac{\alpha_K}{r_K}\ p(x,r,K) = 0\ .$$

Thus,

$$\sum_{i=1}^{N}\left(p(x_i,\beta,m)\ y(x_i) + p(x_i,\ \delta,\ K-1) - p(x_i,\alpha,K)\right)^2 = 0\ .$$

The minimum sum of the squared residuals is zero.

CONCLUDING REMARKS

Rather than using the least squares solution $p(x,\alpha,K)$ as a starting point, the polynomial $p(x,\alpha,K) = x^K$ could be used. This will assure $\alpha_K \neq 0$. However, if the least squares polynomial solution is used as a first attempt to fit the data, then $p(x_i,\alpha,K)$ $i = 1,\ldots,N$, will already be computed to obtain the deviation for the curve. If $\alpha_K \neq 0$ then the rational approximation can be incorporated with the polynomial approximation program. The following procedure has been used satisfactorily. Set K equal to one. Obtain the best least squares fit of degree one. Choose several values of m , say one through five. Obtain the rational approximation for each of these values. This yields several different approximations for one value of K . If these are not acceptable then a range of values for K can be used. The rational approximations should be plotted out at a large number of points between the input data points because of the possibility of singular points.

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